ASC*eNews* - Quarterly Newsletter

December 2010 – NA-ASC-500-10 – Issue 15

Meisner Minute

I hope this quarter's newsletter finds you and your families looking forward to a healthy and prosperous new year. And, professionally, I hope your achievements in the New Year exceed those of a very successful 2010. In spite of presenting you with impediments such as continuing resolutions, your accomplishments are nothing short of amazing. So, I would like to take the time to recount your successes as a challenge for the New Year.

This past year culminated several years of hard work on the Energy Balance knob. For the first time brilliant minds, unprecedented experimental facilities and world-leading simulation capabilities converged at a point in history to solve a fifty-year old scientific challenge. One down, three to go. Not only did you complete the Energy Balance Level 1 milestone, but you also successfully accomplished the objectives outlined in the Forensics Level 1 milestone. Significant improvements in our nuclear properties databases and modeling capabilities support the nation's ability to attribute nuclear events to proliferant groups. Using the unique capabilities of the Nuclear Security Enterprise to serve broader national security needs is a national priority.

The Roadrunner machine reached Critical Decision 4 (CD-4), Operational readiness. This was the first ASC platform to successfully complete the DOE capital acquisition process--starting with CD-0, Mission Need, and proceeding to CD-4--on time and within budget. Even before reaching operational status it made critical contributions to solving Energy Balance. While possibly not as flashy, but no less essential to our achievements, our computing environments continued to mature. Work to date on the TLCC environment allows us to respond to Government Accounting Office's critiques that our contingency operations plans need improvement. Cielo usage model preparations will ensure our capital investments in the Cielo hardware contribute to stockpile stewardship early in the machine's lifecycle.

Speaking of transitioning to Cielo, allow me to close by acknowledging the exceptional accomplishments of Purple. This was the year we decommissioned Purple, the iconic culmination of the ASCI program. While LLNL deserves kudos and can take special pride for successfully carrying-out the immense task engendered in hosting such a machine, the simulation results from all three labs were truly impressive. Purple represents the dawn of an era where scientists and engineers began to speak of simulation as the third leg of science, comparable to theory and experiment, and many of your accomplishments testify to this.

Last year was a pretty impressive year. But, I have learned over a decade with the program not to relax, because there are even harder problems to tackle and more impressive results to achieve. Therein lies motivation and the challenge for the New Year. I look forward with pride to reviewing your achievements this year.

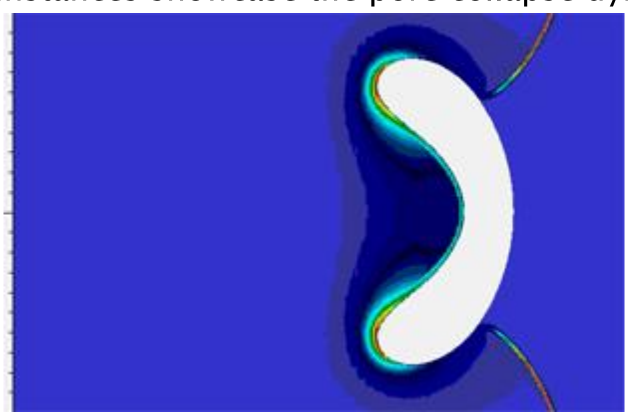
ALE3D Code Simulates 3D Pore Collapse

Understanding the mechanisms of hot-spot initiation in high-explosive (HE) materials is important for the safety, reliability, and development of new insensitive munitions. A computational study at Lawrence Livermore National Laboratory (LLNL) using the code ALE3D investigated the mechanisms of air bubble collapse and hot spot initiation in insensitive high-explosives (IHE).

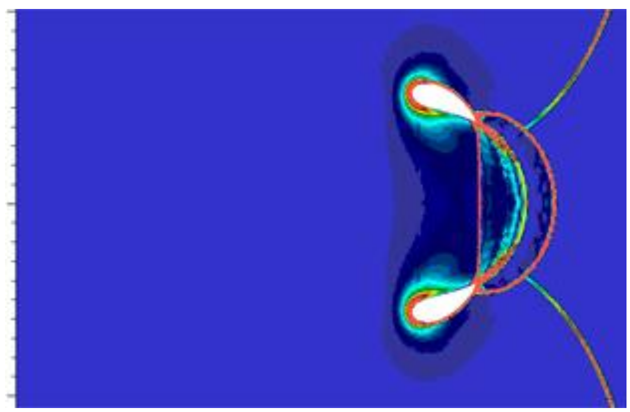
The study focused on non-reactive dynamics to isolate the thermal and hydrodynamics effects. Three-dimensional, high-resolution simulations were performed on the Sequoia Initial Delivery (Dawn) System to evaluate the parallel performance and gain insight on the 3D dynamics of pore collapse. The ALE3D Team completed an initial testing phase for ALE3D using the explicit hydrodynamics and explicit thermal solvers on Dawn. The configuration investigated corresponded to a 3D pore collapse of a spherical air bubble in IHE in support of the ASC's Grain-Scale Simulation Modeling effort (see figure). Several mesh resolutions were considered of 250M and 500M zones, and computations were performed on up to 16,384 Dawn processors.

Solid plastic-bonded HE materials consist of crystals whose size typically ranges between 10 and 100 microns with micron-sized embedded impurities and air bubbles. These voids increase the ease of shock initiation by generating high-temperature regions during their collapse, and these high-temperature regions might lead to ignition of the HE material.

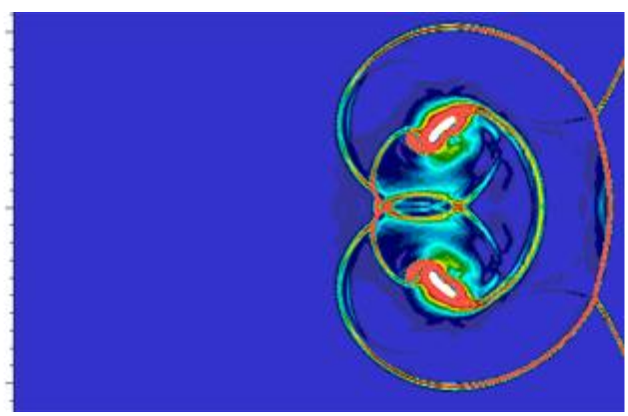
Numerical Schlieren (magnitude of density gradient) contours at three representative time instances showcase the pore collapse dynamics for 2-mm diameter and 25-GPa shock



(a) Pore front wall being pushed toward pore back wall.



(b) Pore collapsing and changing from a spherical shape to a torus.



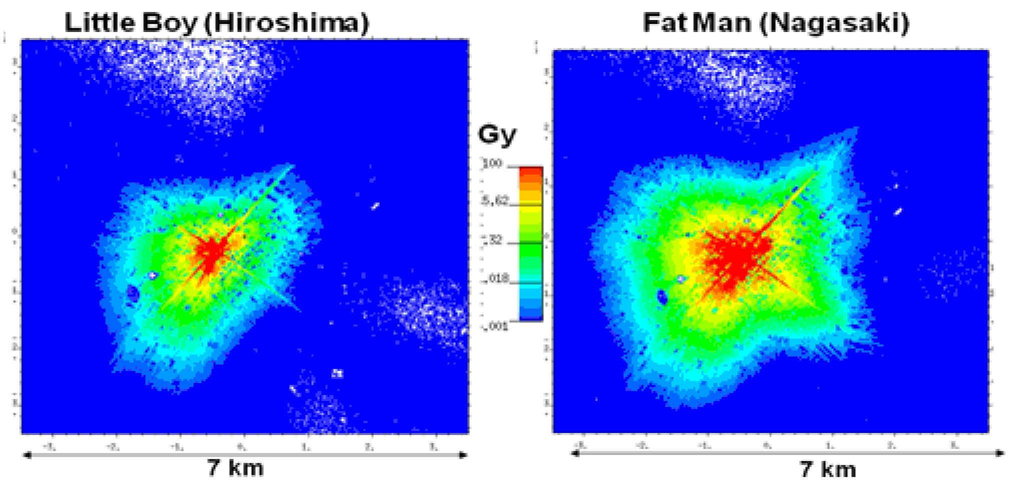
(c) Pore collapsed, rotating, and advecting in IHE, where hot spots can be seen forming in its vicinity.

ASC Simulations Help to Quantify Consequences of Urban Nuclear Detonation

Scientists at Los Alamos National Laboratory (LANL) are working with personnel from the White House Office of Science and Technology Policy (WHOSTP) and the Department of Homeland Security (DHS) to provide assistance to state and local emergency-response planning agencies. They are working together to plan ahead for what can be expected from a possible urban nuclear event. The ASC code, MCNP (a continuous energy Monte Carlo radiation transport code) is being used by LANL scientists to simulate both radionuclide activation of the environment surrounding the event and the prompt radiation and fallout radiation effects on the human population.

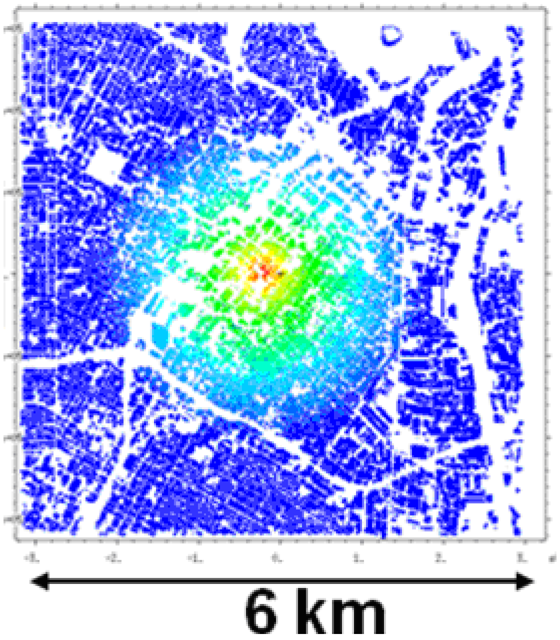
These calculations can incorporate realistic image-based geometries such as buildings, landmasses, vehicles, or any object in the common CAD formats. In a hypothetical detonation of a nuclear weapon, MCNP was used to calculate radiation dose that was then combined with information on population from the US Census databases, including effects such the distribution of people in buildings and on the streets, and the differences of day versus night. The WHOSTP is drafting a policy document with this kind of information to present to DHS in July 2010.

Among its many capabilities, the MCNP code has the ability to calculate weapons-effects information in varying levels of geometric resolution. To resolve a metropolitan area the size of Los Angeles down to a resolution of meters, very large amounts of computer resources are needed. In the future, when exascale computing is a reality, scientists hope to be able to use simulation and analysis to help accomplish real-time evaluation of urban nuclear detonation.



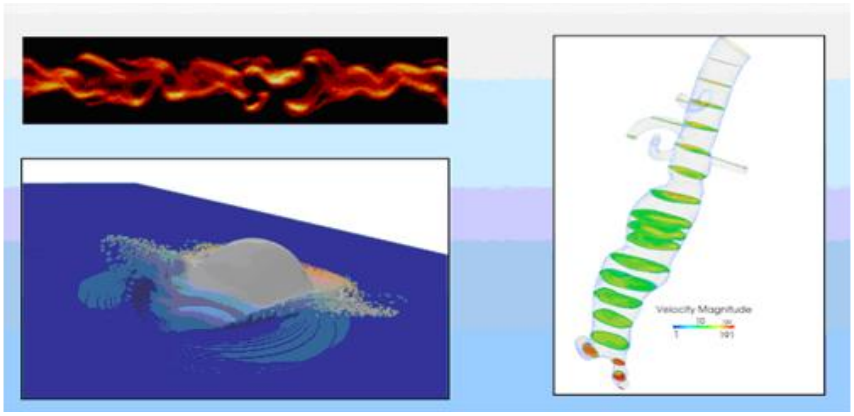
Left: A simulation of nuclear weapon effects (photon dose) in Los Angeles, CA, from two ~20 kilotons (kT) weapons.

Right: Fat Man's photon leakage is 16x higher, resulting in higher dose at distance and greater penetration of buildings. The photon dose is higher than the neutron dose at distance. Some line-of-sight paths have lethal doses ~1.5 km from blast. Note that line-of-sight effects are greater for the leakage photons than for the neutrons, which is why accurate geometry of the buildings is important for determining photon dosage.



Above: Production of the radionuclide Al-28 in cement from Fat Man in Los Angeles, CA. The neutron leakage from Fat Man would cause many elements in the surrounding environment to become radioactive, which becomes a hazard to emergency responders and initial blast survivors, as well as a long-term disposal issue.

ParaView Coprocessing Library Advances High-Fidelity Data Analysis



Images produced by coupling various codes with the ParaView Coprocessing Library, including (clockwise from upper left) Los Alamos National Lab's NPIC, and Rensselaer Polytechnic Institute's PHASTA. The Coprocessing Library can be coupled directly with a code, to perform analysis and visualization of results at runtime. This library has shown strong scaling at up to 32K cores, providing a range of operations such as mesh decimation, slicing, and computing values on a surface. In addition, geometry, images and other data can be written to disk at simulation's native fidelity (one per timestep).

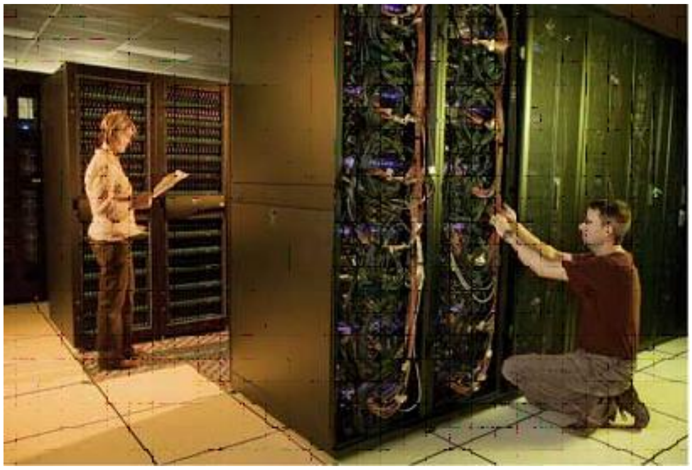
Sandia National Laboratories, in collaboration with Kitware Inc. has delivered the ParaView Coprocessing Library, which advances the state-of-the-art in large scientific data analysis and visualization. This library encapsulates scalable analysis and visualization capability in a high-quality, open-source product.

The science and discoveries in extreme-sized simulations are locked within the enormous data generated on today's Petascale computers, but these data are increasingly difficult to capture because we can calculate data thousands of times faster than we can save it to a disk. This 'information barrier' between what is calculated and what is saved means that we have to be increasingly agile about what data are gleaned from the simulations - requiring that we analyze data while still in the memory on the HPC platform - so we can retain valuable information (features, statistics, and high resolution images) that cannot be captured if we simply wrote raw data to disk.

The ParaView Coprocessing Library provides a technical leap in the ability to break down this 'information barrier' by performing data analysis while the simulation is still running. Using this library, Sandia researchers have demonstrated in-situ data analysis with several running simulations using Sandia National Laboratories' CTH and ALEGRA, Los Alamos National Laboratory's NPIC, and Rensselaer Polytechnic Institute's PHASTA. The ParaView Coprocessing Library has demonstrated excellent scalability when running on over 32,000 processing cores of the Intrepid BlueGene/P at Argonne National Laboratory. More recently, during Supercomputing 2010, a live demo of the ParaView Coprocessing Library visualizing data from a running PHASTA simulation was presented by Argonne National Laboratory.

The ParaView Coprocessing Library is available for download through http://www.paraview.org

Livermore Creates the World's Highest Performance Storage Array



The Hyperion Data Intensive Testbed delivers more than 40,000,000 input/output operations per second and 320 gigbytes per second bandwidth from just two racks of servers. Hyperion was delivered in 2008 but, with the recent addition of the solid-state flash input/output memory, is now at the point where serious operational testing can begin.

From The Wall Street Journal Blog: It's a heady time in high-performance computing, driven by rapid improvements in the chips that supply number-crunching power. The next target could be data storage. | Full Story

From Government Computer News: A prototype computer system is demonstrating the use of flash memory in supercomputing. The Hyperion Data Intensive Testbed at Lawrence Livermore National Laboratory uses more than 100 terabytes of flash memory. | Full Story

From HPCwire: Appro, a leading provider of supercomputing solutions, today announces the deployment of a Data Intensive Testbed Cluster solution based on Appro servers configured with ioMemory technology from Fusion-io to extend the existing Lawrence Livermore National Laboratory Hyperion system. | Full Story

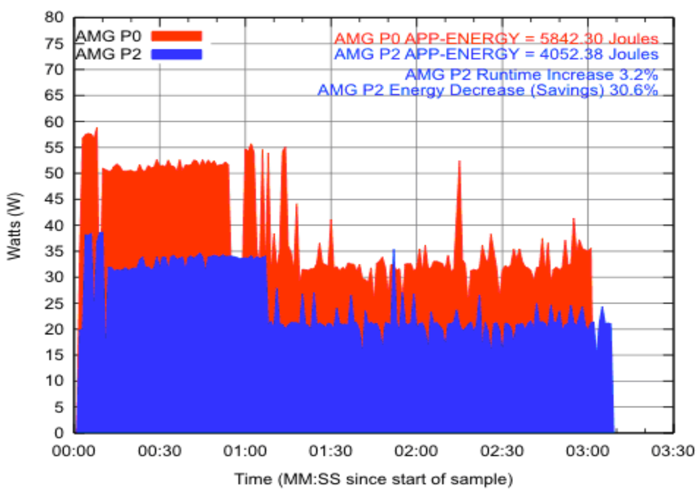
Lowering Energy Use on HPC Systems

Power is now recognized as a critical and potentially limiting factor in architecting current and next generation High Performance Computing (HPC) systems.

Recognizing this issue a number of years ago, Sandia National Laboratories began efforts to investigate and affect power use on HPC platforms beginning with Red Storm.

Our latest efforts have been directed at the energy efficiency of HPC applications at large scale. Commodity hardware and software employ a number of power saving features directed towards extending battery life. Such features could, however, be highly disruptive if used at scale on HPC platforms. Using the advanced monitoring techniques we developed, combined with modifications to our Catamount Light Weight Kernel, we have successfully measured the energy used at scale for the Algebratic Multigrid (AMG) application and a number of other important tri-lab applications while varying the clock frequency of the CPU. By deterministically lowering the CPU frequency, we have successfully taken advantage of the secondary effect of lowering input voltage to the CPU. The dynamic power dissipated by a chip is proportional to the voltage squared. This squared relationship has a much higher impact than the linear relationship resulting from simply lowering the CPU frequency.

The result is shown in the following graph where AMG was first executed at the default CPU frequency (red), and again on the same nodes using a lower CPU frequency (blue). AMG, similar to many other tri-lab applications, is memory bound. Lowering the CPU frequency has the effect of extending run time by 3% but achieves an energy savings of more than 30%, an order of magnitude difference. Further analysis is being conducted on other important tri-lab applications.



This chart shows AMG runtime increased by 3% when running at a lower CPU frequency. But the energy decrease was 30.6%.

Cielo Replaces Purple as ASC Capability Computing Platform

Cielo, (Spanish for sky), is NNSA's next-generation capability computing platform, required by the ASC Program to support the national Stockpile Stewardship Program. Cielo is a Cray Computing system and a project of ACES, the New Mexico Alliance for Computing at Extreme Scale, a joint project of Sandia and Los Alamos national laboratories

Cielo, allocated for ASC's Capability Computing Campaign (CCC) projects, is designed to run simultaneous jobs that use a large percentage of the system resources, although smaller jobs will be accommodated.

With 10 times more peak computing power, Cielo replaces the recently retired ASC Purple system. Installed at Los Alamos, Cielo will support ASC programs at all three NNSA national laboratories beginning Feb. 2011. Cielo will initially provide more than 1 peak petaFLOPS. Consisting of 72 cabinets with a footprint of only 1500 sq. ft., Cielo will use less than 4 megawatts of power for operation.

The Cielo principals are NNSA Federal Project Directors Atinuke Arowojolu and Sander Lee, HQ; ACES Co-Directors Sudip Dosanjh, Sandia National Laboratories (SNL), and John Morrison, Los Alamos National Laboratory (LANL); Project Director Manuel Vigil, LANL; and Chief Architect Doug Doerfler, SNL.

Cielo, NNSA's next-generation capability computing platform. The Cielo system is comprised of 72 cabinets in a 4 x 18 configuration. It is located in the Nicholas Metropolis Center for Modeling and Simulation at LANL.

Cielo (on right side of photo) was featured in the ASC booth at SC10, the international supercomputing conference, held in New Orleans in November.

Purple Supercomputer Fades to Black

From left: Bruce Goodwin (LLNL), Bob Meisner (NNSA), Chris Maher (IBM), and Michel McCoy (LLNL) in the Armadillo theater following the ASC Purple retirement ceremony.

ASC Purple*, the first supercomputer capable of routinely producing the three-dimensional simulations of nuclear weapons performance that underpin stockpile stewardship, was retired in a Terascale Simulation Facility ceremony in November 2010 at Lawrence Livermore National Laboratory.

Delivered in 2005, the IBM Purple machine represented the culmination of the Accelerated Strategic Computing Initiative's (ASCI) nearly 10-year quest to bring online a machine capable of performing 100 teraFLOP/s (trillions of floating point operations per second), regarded by scientists and engineers as the minimum threshold for reliable 3D nuclear weapons performance simulations.

Bob Meisner, NNSA's ASC program director, said that it was Purple that "took the 'i' out of ASCI" and transformed the ambitious initiative into the established program it is today. "Purple was the first machine that provided answers that we could believe in," Meisner said. "The machine proved that high-performance computing could be used as the third leg of science, along with theory and experiment. This was a huge accomplishment."

Bruce Goodwin, principal associate director for Weapons and Complex Integration, lauded the partnership with NNSA and IBM that made Purple possible, recalling that the contract that brought Purple and BlueGene/L to Livermore in 2005 came "on the heels of the Earth Simulator," the Japanese supercomputer ranked No. 1 on the Top500 list at the time.

In one of a number of firsts, Goodwin noted that the Purple system was the first national computational user facility available to scientists and engineers at the three nuclear weapons labs that make up ASC: Los Alamos, Sandia and Lawrence Livermore national labs.

"Purple was an iconic system. The goal of ASCI was to demonstrate an entry-level ability to run an integrated design calculation in 3D. This was achieved even as the machine was integrated," Goodwin said. "What is not as widely recognized is that this triumph was overshadowed by an even greater accomplishment: calculations that paved the way for the reorientation of the weapons program towards predictive simulation. Purple stood for both an end and a beginning and a computer can have no greater epitaph than this."

Purple was th1e last of a distinguished class of IBM supercomputers dedicated to the nuclear weapons program, a class that included ASCI Blue Pacific and White.

Goodwin said Purple's capabilities "have changed the world" in high-performance scientific computing and led to the discovery of new science and new physics. Phenomena revealed by Purple simulations made the "thermonuclear boost initiative possible."

*View the ASC Purple Web site for a video commemorating the now-retired supercomputer.

Roadrunner Successfully Transitions into Secure Computing

Soon after it was accredited for full operations in the classified computing environment, users of the Roadrunner supercomputer located at Los Alamos National Laboratory (LANL) were ready to go with many applications that have been customized for Roadrunner's cell processors. Large-scale weapon science calculations are already proving to be an important use of the Roadrunner capabilities in the classified environment. A seasoned user of ASC platforms since the inception of ASC, Bob Weaver remarks after running on Roadrunner since January 2010, "I am extremely impressed with the performance of the cell-based algorithm. There is significant opportunity for the resolution of several outstanding weapons physics issues."

Weaver and team ran initial calculations to evaluate the speedup provided by the cell-based algorithm over a comparable algorithm that uses only the opteron processors. The comparison showed that the cell-based work was uniformly approximately 10X faster than the opteron algorithm on real problems of interest. Given this improved performance, the team is able to use the cell-based algorithm in place of a previous coarse approximation in their everyday work and realize a tremendous improvement in physics fidelity with only a slight (10%) increase in turn-around time.

The integration of ASC, Science Campaigns, and Directed Stockpile Work has enabled ASC codes to become the standard basis for weapons baselines, annual certification, peer review, SFIs, and LEPs.

New Applied Computer Science Group Created

Above, Sriram Swaminarayan, Group Leader for the Applied Computer Science Group, collaborating with scientists at LANL.

Being at the heart of the nation's computational science advances, computational scientists in the Los Alamos National Laboratory's (LANL's) ASC Program are leveraging their unique experience with hybrid computing (built over many years leading up to Roadrunner) to create applications of the future. A new group at LANL is pairing these scientists with weapons program scientists to focus on easing the transition of nuclear weapons applications onto next-generation architectures.

The Applied Computer Science Group is addressing scientific applications at extreme scale, through co-design of applications and algorithms, innovation in programming models, collaborative programming and code development, and exploration of data science at scale. This group will play an increasingly important role for the ASC Program as the simulation capabilities supporting the stockpile stewardship program evolve to the future of computing at the extreme scale.

The group members are also building momentum in the external community through partnerships with other national laboratories and memberships in appropriate standards bodies to guide future tool development. For example, this team founded the Hybrid Multicore Consortium and is a member of Khronos Group, the governing body of OpenCL.

Supercomputing 2010 Booth Acknowledges the Past and Focuses on the Future

Three 14-foot towers showed life-sized scientists immersed in their research. Clear plexiglass plaques featured text describing the science. On the other side of the towers, contributors used laptops to demonstrate their work to conference attendees.

Every year, the NNSA ASC Program sponsors a booth in the exhibition hall at the Supercomputing Conference, where leading researchers and industry vendors worldwide showcase the latest high performance computing (HPC), networking, storage, and analysis products and innovations. The theme for this year's ASC booth-Where Discoveries Advance National Security-set the tone for a "3D" design that both showed ASC scientists "stepping into" their areas of expertise while allowing visitors to "step into" five of the ASC supercomputers. The booth was part of the Supercomputing 2010 conference, held Nov. 13-19 in New Orleans.

The Advanced Systems wall behind the reception desk invited conference attendees to "enter" the booth and the machine room floor. Clear plexiglass plaques featured descriptions of the three advanced systems machines.

"The ASC booth at Supercomputing allows NNSA to showcase its unique expertise in supercomputing in the interest of national security," said Bob Meisner, ASC program director at NNSA Headquarters in Washington, D.C. "Over the years, ASC has paved the way for new scientific discoveries and research, along with cutting-edge HPC hardware and software advancements."

Technical staff from Los Alamos, Sandia, and Lawrence Livermore national laboratories contributed to various forums at the conference, including: 13 posters, 5 technical papers, and 5 tutorials. They participated in 2 panels and 6 "birds-of-a-feather" sessions. Dona Crawford, Computation Associate Director for Lawrence Livermore, participated in the panel discussion entitled "Return of HPC Survivor: Outwit, Outlast, Outcompete." Salman Habib, a researcher from Los Alamos, contributed "Computing the Universe," a masterworks presentation, which is an invited presentation that highlights innovative ways of applying HPC to the world's most challenging problems.

The Capability Systems wall explored the concept of "workhorse" in the context of the ASC Purple and Cielo machines. Purple retired this November, and Cielo, located at LANL, will become the new ASC workhorse machine.

To bring the booth alive for conference attendees, scientists and researchers from the three labs contributed simulations and research, and made presentations to bring the booth alive for conference attendees. This year, the booth featured three towers to represent the three defense aspects of the ASC Program: Integrated Codes, Physics and Engineering Models, and Verification and Validation. In addition, two booth walls featured the ASC supercomputers: one wall for the Advanced Systems (Sequoia, Hyperion, and Roadrunner), and one wall for the Capability Systems (the retiring Purple and the incoming Cielo machines). The following images show the ASC booth.

Lawrence Livermore Hosts HPC Best Practices Workshop on Power Management

Participants from more than 25 high performance computing (HPC) organizations and commercial vendors joined representatives from several government agencies for a workshop on HPC best practices that was held Sept. 28-29 in San Francisco. The workshop purpose was to identify best practices related to power management at HPC centers. It was hosted by LLNL on behalf of NNSA and the Office of Science. This by-invitation workshop was the fourth in a series of DOE HPC Best Practices workshops. Previous workshops addressed system integration, risk management, and software lifecycles.

Power management has been identified as a key issue for future systems-especially exascale systems. Sessions addressed the current practices and issues related to controlling and reducing power required by facilities and systems. Alternative and green energy solutions were also discussed.

More information about the workshop can be found at the workshop Web site. Presentations and breakout session reports can also be accessed from the Web site. A "birds of a feather" session at SC10 reported on the key findings from the workshop.

LLNL Hosts U.S. and U.K. Labs at JOWOG 34

JOWOG 34, the Joint Operations Weapons Operations Working Group for information technology in weapons systems, was held May 17-21 at LLNL. JOWOG 34 is an annual meeting of information technology and high-performance computing (HPC) staff from the three NNSA laboratories and the United Kingdom's Atomic Weapons Establishment (AWE). The JOWOG meetings were established in 1958 to facilitate the exchange of ideas between nuclear laboratories in the U.S. and the U.K.

This year, the working group included more than 50 presentations from the four laboratories on topics including long-term HPC strategy, HPC capability and capacity systems, desktop systems and support, performance, visualization, and security. There were extensive discussions of strategies for future exascale procurements and updates on current petascale procurements, including the Sequoia machine at LLNL. JOWOG 34 also included a special workshop on HPC architectural simulation and modeling, which is used by the laboratories to guide future procurements. Guests were given tours of the National Ignition Facility and the Terascale Simulation Facility machine room.

Lab Physicist Honored for Work at Department of Energy Headquarters

NNSA Administrator Tom D'Agostino, left, and DOE Undersecretary for Science Steve Koonin, right, award LLNL's Kim Budil the NNSA Administrator's Award for Excellence Medal.

Kim Budil, an LLNL physicist on assignment in Washington D.C. to the NNSA, has received a rarely bestowed honor, the NNSA Administrator's Award for Excellence Medal, for distinguished service in the national security interests of the United States.

Budil had been working in the Weapons and Complex Integration (WCI) Directorate and in association with the ASC Program, when she was selected a year-and-a-half ago by the Department of Energy's Undersecretary for Science, Steve Koonin, to serve as a senior adviser on science related to national security.

Budil was praised for her keen ability to work effectively with people. Among her assignments was developing an agenda and organizing a two-day senior review with external experts for Koonin and NNSA Administrator Tom D'Agostino, about the nuclear weapons stockpile and the technical skills needed to sustain it. She worked with leaders of Los Alamos and Lawrence Livermore national laboratories to help them deliver appropriate and succinct presentations to the reviewers. Following those presentations, she assisted in preparing a summary that was designed to start a senior-level discussion headed by Energy Secretary Chu and Presidential Science Adviser John Holdren.

Budil's other activities included technical workshop preparations, integrating materials science interests at DOE, organizing a review by the National Academy of Sciences on Inertial Fusion Energy and organizing Koonin's review of the National Ignition Campaign.

"In 27 years of federal service at the Department of Energy, I have never had a better working relationship than I have had with Kim Budil," said David Crandall, NNSA's chief scientist. "In every situation she has been able to sense what people need and to astutely apply technical analysis that addresses the questions."

In presenting the medal to Budil, D'Agostino pointed out that the honor is rarely given to someone on a short-term assignment to NNSA. He praised her for advancing awareness of DOE and NNSA science and technology capabilities at the national labs and for effectively forwarding NNSA and Office of Science interests and expertise.

According to Crandall, "Most importantly, she earned trust and respect of all three undersecretaries: Koonin, D'Agostino and (Kristina) Johnson and the Deputy Secretary, Dan Poneman. All of them engaged Kim on technical topics that needed accuracy and personal savvy as to what was needed by them."

Budil will return to LLNL when her assignment ends in December.

ASC Relevant Research

Sandia National Laboratories
Citations for Publications in 2010

1. Alvin, K., Barrett, B., Brightwell, R., Dosanjh, S., Geist, A., Hemmert, K. S., Heroux, M., Kothe, D., Murphy, R., Nichols, J., Oldfield, R., Rodrigues, A., Vetter, J. (2010). "On the Path to Exascale," International Journal of Distributed Systems and Technologies, Vol. 1, No. 2, pp. 1-22.
2. Ang, J., Brightwell, R., Dosanjh, S., et al. (to be published). "Exascale Computing and the Role of Co-design," Book Chapter, Springer-Verlag.
3. Ang, J., Doerfler, D., Dosanjh, S., Koch, K., Morrison, J.,Vigil, M. (2010). "The Alliance for Computing at the Extreme Scale," Proceedings, Cray Users Group Meeting, Edinburgh, Scotland.
4. Brandt, J., Chen, F., De Sapio, V., Gentile, A., Mayo, J., Pébay, P., Roe, D., Thompson, D., Wong, M. (2010). "Quantifying Effectiveness of Failure Prediction and Response in HPC Systems: Methodology and Example," Proceedings, IEEE/IFIP International Conference on Dependable Systems and Networks, International Workshop on Fault-Tolerance for HPC at Extreme Scale, Chicago, Illinois.
5. Brandt, J., Chen, F., De Sapio, V., Gentile, A., Mayo, J., Pébay, P., Roe, D., Thompson, D., Wong, M. (2010). "Using Cloud Constructs and Predictive Analysis to Enable Pre-Failure Process Migration in HPC Systems" Proceedings, IEEE International Symposium on Cluster, Cloud, and Grid Computing, Workshop on Resiliency in High-Performance Computing in Clusters, Clouds, and Grids, Melbourne, Australia.
6. Brandt, J., Chen, F., De Sapio, V., Gentile, A., Mayo, J., Pébay, P., Roe, D., Thompson, D., Wong, M. (2010) "Combining Virtualization, Resource Characterization, and Resource Management to Enable Efficient High Performance Compute Platforms Through Intelligent Dynamic Resource Allocation" Proceedings, IEEE International Parallel and Distributed Processing Symposium, Workshop on System Management Techniques, Processes, and Services, Atlanta, Georgia.
7. Brightwell, R. (2010). "Exploiting Direct Access Shared Memory for MPI on Multi-Core Processors," International Journal of High Performance Computing Applications, Vol. 24, pp. 69-77.
8. Brightwell, R., Ferreira, K., Riesen, R. (2010). "Transparent Redundant Computing with MPI," Proceedings, European MPI Users Group Conference, Stuttgart, Germany.
9. Curry, M., Ward, L., Skjellum, A., Brightwell, R. (2010). "A Lightweight, GPU-Based Software RAID System," Proceedings, International Conference on Parallel Processing, San Diego, CA.
10. Dongarra, J. et al. (2011). "The International Exascale Software Project Roadmap," International Journal of High Performance Computing Applications, 25:1, 2011.
11. Ferreira, K., Bridges, P., Brightwell, R., Pedretti, K. (2010). "The Impact of System Design Parameters on Application Noise Sensitivity," Proceedings, IEEE International Conference on Cluster Computing, Crete, Greece.
12. Hemmert, K. S., Barrett, B., Underwood, K. (2010). "Using Triggered Operations to Offload Collective Communication Operations," Best Paper Session (**) Proceedings, European MPI Users Group Conference, Stuttgart, Germany.
13. Hsieh, M., Thompson, K., Song, W., Rodrigues, A., Riesen, R. (2010). "A Framework for Architecture-level Power, Area and Thermal Simulation and its Application to Network-on-chip Design Exploration," 1st International Workshop on Performance Modeling, Benchmarking and Simulation of High Performance Computing Systems (PMBS 10) at the SC10, New Orleans, Louisiana.
14. Hu, S., Murphy, R., Dosanjh, S., Olukoton, R., Poole, S. (2010). "Hardware/Software Co-Design for High Performance Computing," Proceedings, CODES+ISSS '10, Scottsdale, Arizona.
15. Jensen, D., Rodrigues, A. (2010). "Embedded Systems and Exascale Computing" Computing in Science And Engineering. November/December 2010, Volume 12, Num. 6.

16. Johnson, C., Bunde, D., Leung, V., (2010). "A Tie-Breaking Strategy for Processor Allocation in Meshes," Proceedings, International Workshop on Scheduling and Resource Management for Parallel and Distributed Systems, San Diego, California.
17. Lange, J., Pedretti, K., Hudson, T., Dinda, P., Cui, Z., Xia, L., Bridges, P., Gocke, A., Jaconette, S., Levenhagen, M., Brightwell. R. (2010). "Palacios and Kitten: New High Performance Operating Systems for Scalable Virtualized and Native Supercomputing," Proceedings, International Parallel and Distributed Processing Symposium, Atlanta, Georgia.
18. Leung, V., Sabin, G., Sadayappan, P. (2010). "Parallel Job Scheduling Policies to Improve Fairness - A Case Study," Proceedings, International Workshop on Scheduling and Resource Management for Parallel and Distributed Systems, San Diego, California.
19. Lofstead, J., Zheng, F., Liu, Q., Klasky, S., Oldfield, R., Kordenbrock, T., Schwan, K., Wolf, M., "Managing Variability in the IO Performance of Petascale Storage Systems," Proceedings, ACM/IEEE Conference on High Performance Networking and Computing (SC10), New Orleans, Louisiana.
20. Pébay, P., Thompson, D., Bennett, J. (2010). "Computing Contingency Statistics in Parallel: Design Trade-Offs and Limiting Cases" Proceedings, IEEE International Conference on Cluster Computing, Crete, Greece.
21. Rodrigues, A., Cook, J., Cooper-Balis, E., Hemmert, K. S., Kersey, C., Riesen, R., Rosenfeld, P., Oldfield, R., Weston, M., Jacob, B., Barrett, B. "The Structural Simulation Toolkit," 1st International Workshop on Performance Modeling, Benchmarking and Simulation of High Performance Computing Systems (PMBS 10) at the SC10, New Orleans, Louisiana.
22. Rodrigues, A., Dosanjh, S. Hemmert, K. S. (2010). "Co-design for High Performance Computing," Proceedings, International Conference on Numerical Analysis and Applied Mathematics, Rhodes, Greece.
23. Shalf, J., Dosanjh, S., Morrison, J. (2010) "Exascale Technology Challenges," to published in VECPAR'10 post-conference book, Berkeley, California.
24. Stearley, J., Corwell, S. Lord, K. (2010). "Bridging the Gaps: Joining Information Sources with Splunk", USENIX Workshop on Managing Systems via Log Analysis and Machine Learning Techniques, Vancouver, BC, Canada.
25. Tomkins, J., Brightwell, R., Camp, W., Dosanjh, S., Kelly, S., Lin, P., Vaughan, C., Levesque, J., Tipparaju. V. (2010). "The Red Storm Architecture and Early Experiences with Multi-core Processors," International Journal of Distributed Systems and Technologies, Vol. 1, No. 2, pp. 74-93.
26. Vaughan, C., Rajan, M., Doerfler, D., Barrett, R. (2010). "From Red Storm to Cielo: Performance Analysis of ASC Simulation Programs Across an Evolution of Multicore Architectures," Poster, ACM/IEEE Conference on High Performance Networking and Computing (SC10), New Orleans, Louisiana.
27. Walker, P., Bunde, D., Leung, V. (2010). "Faster High Quality Processor Allocation," Proceedings, Linux Cluster Institute International conference on High-Performance Cluster Computing, Pittsburg, Pennsylvania.

Citations for Publications in 2009

1. Barrett, B., Hemmert, K. S. (2009). "An Application Based MPI Message Throughput Benchmark," Proceedings, IEEE International Conference on Cluster Computing, New Orleans, Louisiana.
2. Bennett, J., Pébay, P., Roe, D., Thompson D. (2009)."Numerically Stable, Single-Pass, Parallel Statistics Algorithms," Proceedings, IEEE International Conference on Cluster Computing, New Orleans, Louisiana.
3. Brandt, J., Gentile, A., Mayo, J., Pébay, P., Roe, D., Thompson, D., Wong, M. (2009). "Methodologies for Advance Warning of Compute Cluster Problems via Statistical Analysis: A Case Study," Proceedings, ACM International Symposium on High Performance Distributed Computing, Workshop on Resiliency in High Performance Computing, Munich Germany.

4. Brandt, J., Gentile, A., Mayo, J., Pébay, P., Roe, D., Thompson,D., Wong, M. (2009). "Resource Monitoring and Management with OVIS to Enable HPC in Cloud Computing," Proceedings, IEEE International Parallel and Distributed Processing Symposium, Workshop on System Management Techniques, Processes, and Services, Rome, Italy.
5. Brightwell, R., Heroux, M., Wen, Z., Wu. J. (2009). "Parallel Phase Model: A Programming Model for High-end Parallel Machines with Manycores," Proceedings, International Conference on Parallel Processing, Vienna, Austria.
6. Laros, J., Pedretti, K., Kelly, S., Van Dyke, J., Ferreira, K., Vaughan, C., Swan, M. (2009). "Topics on Measuring Real Power Usage on High Performance Computing Platforms,", Proceedings, IEEE International Conference on Cluster Computing, New Orleans, Louisiana.
7. Laros, J., Pedretti, K., Kelly, S., Van Dyke, J., Ferreira, K., Vaughan, C., Swan, M. (2009). "Investigating Real Power Use on Red Storm," Proceedings, Cray Users Group Meeting, Atlanta, Georgia.
8. Leon, E., Riesen R., Maccabe, A. B., Bridges, P. (2009). "Instruction-Level Simulation of a Cluster at Scale," Proceedings, IEEE/ACM International Conference on High-Performance Computing, Networking, Storage, and Analysis (SC09), Portland, OR.
9. Underwood, K., Brightwell, R., Hemmert, K. S. (2009). "Chapter 5 - Network Interfaces for High-Performance Computing,"Attaining High Performance Communication: A Vertical Approach, CRC Press.
10. Underwood, K, Hemmert, K. S., Ulmer, C. (2009). "From Silicon to Science: The Long Road to Production Reconfigurable Supercomputing," ACM Transactions on Reconfigurable Technology and Systems, Vol. 2, No. 3.
11. Wheeler, Thain, D., Murphy R., "Portable Performance from Workstation to Supercomputer: Distributing Data Structures with Qthreads," Proceedings, First Workshop on Programming Models for Emerging Architectures, Raleigh, North Carolina.

Los Alamos National Laboratory
Citations for Publications in 2010

1. Aslam, T.D., et al. (2010). "PROTON RADIOGRAPHY OF PBX 9502 DETONATION SHOCK DYNAMICS CONFINEMENT SANDWICH TEST," in AIP Conference Proceedings, 2 HUNTINGTON QUADRANGLE, STE 1NO1, MELVILLE, NY 11747-4501 USA, pp. 241-244.
2. Chisolm, E.D., et al. (2010). "SHOCK HUGONIOTS OF MOLECULAR LIQUIDS AND THE PRINCIPLE OF CORRESPONDING STATES," in AIP Conference Proceedings, 2 HUNTINGTON QUADRANGLE, STE 1NO1, MELVILLE, NY 11747-4501 USA, pp. 556-559.
3. Colgan, J., et al. (2010). "Non-LTE studies of boron plasma," JOURNAL OF PHYSICS B-ATOMIC MOLECULAR AND OPTICAL PHYSICS, vol. 43, p. 144021.
4. Crockett, S.D. and C.W. Greeff (2010). "A GALLIUM MULTIPHASE EQUATION OF STATE," in AIP Conference Proceedings, 2 HUNTINGTON QUADRANGLE, STE 1NO1, MELVILLE, NY 11747-4501 USA, pp. 1191-1194.
5. Densmore, J.D., et al.(2010). "Stability analysis and time-step limits for a Monte Carlo Compton-scattering method," JOURNAL OF COMPUTATIONAL PHYSICS, vol. 229, pp. 3691-3705.
6. Dimonte, G. (2010). "A cell kinetics model for prostate cancer and its application to clinical data and individual patients," JOURNAL OF THEORETICAL BIOLOGY, vol. 264, pp. 420-442.
7. Feagin, J.M., et al. (2010). "Electron-pair excitations and the molecular coulomb continuum," in Journal of Physics: Conference Series, UK, p. 022053 (1 pp.).
8. Greeff, C.W., et al. (2010). "THE COLD EQUATION OF STATE OF TANTALUM," in AIP Conference Proceedings, 2 HUNTINGTON QUADRANGLE, STE 1NO1, MELVILLE, NY 11747-4501 USA, pp. 681-684.

9. Grove, J.W. (2010). "PRESSURE-VELOCITY EQUILIBRIUM HYDRODYNAMIC MODELS," ACTA MATHEMATICA SCIENTIA, vol. 30, pp. 563-594.
10. Hansen, B.L., et al. (2010). "Dislocation subgrain structures and modeling the plastic hardening of metallic single crystals," Modelling and Simulation in Materials Science and Engineering, vol. 18, p. 055001.
11. Hammerberg, J.E., et al.(2010). "HIGH VELOCITY PROPERTIES OF THE DYNAMIC FRICTIONAL FORCE BETWEEN DUCTILE METALS," in AIP Conference Proceedings, 2 HUNTINGTON QUADRANGLE, STE 1NO1, MELVILLE, NY 11747-4501 USA, pp. 777-780.
12. Huzurbazar, A.V., and B.J. Williams (2010). "Incorporating Covariates in Flowgraph Models: Applications to Recurrent Event Data," TECHNOMETRICS, vol. 52, pp. 198-208.
13. Lloveras, P., et al. (2010). "Thermodynamics of stress-induced ferroelastic transitions: Influence of anisotropy and disorder," PHYSICAL REVIEW B, vol. 81, p. 214105.
14. Menikoff, R. (2010). "ON BEYOND THE STANDARD MODEL FOR HIGH EXPLOSIVES: CHALLENGES & OBSTACLES TO SURMOUNT," in AIP Conference Proceedings, 2 HUNTINGTON QUADRANGLE, STE 1NO1, MELVILLE, NY 11747-4501 USA, pp. 18-25.
15. Monroe, L. and D. Pugmire (2010). "A case study of collaborative facilities use in engineering design," in Proceedings of the SPIE - The International Society for Optical Engineering, USA, p. 752509 (8 pp.).
16. Németh, K., et al. (2010). "The choice of internal coordinates in complex chemical systems," Journal of Computational Chemistry, vol. 31, pp. 2078-2086.
17. Pindzola, M.S., et al. (2010). "Electron-impact ionization of C-2," JOURNAL OF PHYSICS B-ATOMIC MOLECULAR AND OPTICAL PHYSICS, vol. 43, p. 065201.
18. Pindzola, M.S., et al. (2010). "Photoionization of highly charged atomic ions," PHYSICAL REVIEW A, vol. 81, p. 063431.
19. Rudin, S.P. (2010). "Alternating layers of plutonium and lead or indium as surrogate for plutonium," IOP Conference Series: Materials Science and Engineering, vol. 9, p. 012098 (8 pp.).
20. Sancho, J.C., et al. (2010). "Analyzing the Trade-off between Multiple Memory Controllers and Memory Channels on Multi-core Processor Performance," in 2010 IEEE International Symposium on Parallel & Distributed Processing, Workshops and Phd Forum (IPDPSW 2010); 19-23 April 2010; Atlanta, GA, USA, Piscataway, NJ, USA, p. 7 pp.
21. Scovel, C.A. and R. Menikoff (2010). "A VERIFICATION AND VALIDATION EFFORT FOR HIGH EXPLOSIVES AT LOS ALAMOS NATIONAL LAB," in AIP Conference Proceedings, 2 HUNTINGTON QUADRANGLE, STE 1NO1, MELVILLE, NY 11747-4501 USA, pp. 169-172.
22. Shaw, M.S., et al. (2010). "OPTIMIZED NESTED MARKOV CHAIN MONTE CARLO SAMPLING: APPLICATION TO THE LIQUID NITROGEN HUGONIOT USING DENSITY FUNCTIONAL THEORY," in AIP Conference Proceedings, 2 HUNTINGTON QUADRANGLE, STE 1NO1, MELVILLE, NY 11747-4501 USA, pp. 529-532.
23. Triplett, B.S., et al.(2010). "DEVELOPMENT OF AN AUTOMATED TESTING SYSTEM FOR VERIFICATION AND VALIDATION OF NUCLEAR DATA AND SIMULATION CODE," NUCLEAR TECHNOLOGY, vol. 170, pp. 80-89.
24. Wallace, D.C., et al. (2010). "Statistical mechanics model for the transit free energy of monatomic liquids," PHYSICAL REVIEW E, vol. 81, p. 041201.
25. Watanabe, T., et al. (2010). "Calculation of prompt fission product average cross sections for neutron-induced fission of U 235 and Pu 239," Journal of Nuclear Science and Technology, vol. 47, pp. 470-481.

Citations for Publications in 2009

1. Azhgirey, I.L., et al. (2009). "CTOF measurements and Monte Carlo analyses of neutron spectra for the backward direction from an iron target irradiated with 400-1200 MeV protons," NUCLEAR INSTRUMENTS & METHODS IN PHYSICS RESEARCH SECTION B-BEAM INTERACTIONS WITH MATERIALS AND ATOMS, vol. 267, pp. 3601-3605.

2. Chandler, C.F., et al. (2009). "Towards resilient high performance applications through real time reliability metric generation and autonomous failure correction," in 2009 Workshop on Resiliency in High Performance, Resilience'09, Co-located with the 2009 International Symposium on High Performance Distributed Computing Conference, HPDC'09; 20090609 - 20090609; Garching, Germany, 1515 Broadway, 17th Floor New York, NY 10036-5701, United States, pp. 1-6.
3. Dai, W.W., and P.R. Woodward (2009). "Multi-dimensional High-order Numerical Schemes for Lagrangian Hydrodynamics," in 2009 International Conference on Scientific Computing. CSC 2009; 13-16 July 2009; Las Vegas, NV, USA, Las Vegas, NV, USA, pp. 213-19.
4. Densmore, J.D. (2009). "Asymptotic Analysis of Spatial Discretizations in Implicit Monte Carlo: Extension to a Courant Time-Step Limit," Transactions of the American Nuclear Society, vol. 101, pp. 437-40.
5. Fichtl, E.D., et al. (2009). "Uncertainty Quantification in Radiation Transport Using the Stochastic Collocation Method," Transactions of the American Nuclear Society, vol. 101, pp. 1106-7.
6. Harris, A.L., et al. (2009). "Four-body model for transfer excitation," PHYSICAL REVIEW A, vol. 80, p. 062707.
7. Henning, P., et al. (2009). "TRAILBLAZING WITH ROADRUNNER," COMPUTING IN SCIENCE & ENGINEERING, vol. 11, pp. 91-95.
8. Hogden, J. (2009). "A Blind Algorithm for Recovering Articulator Positions from Acoustics," in 2009 43rd Asilomar Conference on Signals, Systems and Computers; 1-4 Nov. 2009; Pacific Grove, CA, USA, Piscataway, NJ, USA, pp. 1737-41.
9. Holmstrom, E., et al. (2009). "Ab initio method for locating characteristic potential-energy minima of liquids," PHYSICAL REVIEW E, vol. 80, p. 051111.
10. Pereira, J., et al. (2009). "Beta-decay half-lives and beta-delayed neutron emission probabilities of nuclei in the region A less than or similar to 110, relevant for the r process," PHYSICAL REVIEW C, vol. 79, p. 035806.
11. Souvatzis, P., et al. (2009). "Dynamical stabilization of the body centered cubic phase in lanthanum and thorium by phonon-phonon interaction," JOURNAL OF PHYSICS-CONDENSED MATTER, vol. 21, p. 175402.
12. Wallace, D.C., et al. (2009). "Improved model for the transit entropy of monatomic liquids," PHYSICAL REVIEW E, vol. 79, p. 051201.

ASC Salutes Christine Wu

Behind the scenes of the ASC Program, Scientist Christine Wu works as a staff member of the Equation of State and Materials Theory Group at Lawrence Livermore National Laboratory.

"What I enjoy most about my job is the creative process of exploring unknowns and gaining new insight," said Christine. She studies materials behavior and equation of state properties using high performance computers. Her specialty is studying materials such as metals and high explosives under extreme conditions relevant to stockpile science, using simulation methods involving individual atoms and molecules.

"What I strive to do is go beyond reproducing experiments. I work hard to figure out what the large amount of simulation data tell us," said Christine. "I use the ASC simulation tools to study physical and chemical properties of materials and discover novel behavior. I am attracted to controversial problems. To me, an unsolved mystery often signals something new and important, and I try to figure out why."

Consider, for example, melting of a metal under pressure, where a significant controversy remains. Dramatically different melting lines are frequently obtained from the two major high-pressure experimental techniques. One technique, using laser-heated diamond-anvil cells (DAC), often yields melting temperatures thousands of degrees lower than measurements by the other technique, which uses shock-waves. Which melt curve should one believe? Resolving this problem has spawned a decade-long active debate within the scientific community.

Christine and her colleagues have proposed a novel resolution. Their research on tantalum was recently featured in Nature Materials magazine in an article entitled "Shear-Induced Anisotropic Plastic Flow from Body-Centred-Cubic Tantalum before Melting." Using simulations, they discovered that crystalline tantalum undergoes viscous plastic flow under shear and heating near the "low" DAC melt line. The viscous flow state shares many similarities with a liquid, giving the appearance of a liquid except with no liquid-like atomic diffusion. If confirmed, this non-equilibrium novel state of matter will have wide scientific importance and engineering implications, including understanding the earth's interior.

"Our findings demonstrated the importance of looking beyond thermodynamically stable phases when explaining unconventional phenomena observed in high-pressure experiments," said Christine. "We need to understand the effect of kinetics. As we have shown in this work, shear does play an important role in materials properties under high pressure."

Link for Nature Materials article:
http://www.nature.com/nmat/journal/v8/n3/full/nmat2375.html